

Journal of Magnetic Resonance

EDITOR: Wallace S. Brey, Jr.

EDITORIAL BOARD:

E. Raymond Andrew	David M. Grant	Ralph Livingston
Edwin D. Becker	R. K. Harris	Bruce McGarvey
A. David Buckingham	K. H. Hausser	Rex E. Richards
S. M. Castellano	Paul S. Hubbard	Max T. Rogers
B. P. Dailey	Charles S. Johnson, Jr.	Thomas A. Scott
P. Diehl	J. Jonas	Bernard L. Shapiro
Richard Ernst	Masaji Kubo	J. B. Stothers
Ray Freeman	George C. Levy	Robert L. Vold

Volume 22, 1976



ACADEMIC PRESS
New York and London

A Subsidiary of Harcourt Brace Jovanovich, Publishers

Copyright © 1976 by Academic Press, Inc.

ALL RIGHTS RESERVED

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

Made in Great Britain

CONTENTS OF VOLUME 22

NUMBER 1, APRIL 1976

SLAWOMIR SZYMAŃSKI AND ADAM GRYFF-KELLER. Analysis of DNMR Lineshape by an Iterative Least-Squares Method	1
V. P. CHACKO AND P. T. MANOHARAN. Forbidden Hyperfine Lines in the EPR Spectra of a Low-Spin Cobalt (II) Complex	7
MICHAEL K. BOWMAN, HIROTOMO HASE, AND LARRY KEVAN. Saturation Behavior of Inhomogeneously Broadened EPR Lines Detected with Magnetic Field Modulation	23
N. C. HALDER. Temperature Dependence of Nuclear Quadrupolar Relaxation Rate in Liquid Metals	33
R. BAR-ADON, S. SCHLICK, H. GILBOA, AND BRIAN L. SILVER. Molecular Motion in a Solid Propellane	41
M. HOLZ, R. B. JORDAN, AND M. D. ZEIDLER. Cd-113 Nuclear Magnetic Relaxation in Aqueous Cadmium Perchlorate Solutions	47
A. ABRAGAM, V. BOUFFARD, AND Y. ROINEL. Concentration, Relaxation, and Phonon Bottleneck of Paramagnetic Centers: A New Experimental Method of Study	53
M. P. EASTMAN, C. D. JAEGER, D. A. RAMIREZ, S. L. KELLY, AND P. W. PERCIVAL. ESR Studies of Valinomycin Ion Pair Complexes	65
VALENTIN S. DIMITROV. Dynamic NMR: Integral Parameter Sensitivities and Their Use in the Total Lineshape Analysis	71
WILSON M. GULICK, JR., GRACE L. SWARTZ, AND ROB G. PARRISH. Carbon-13 Hyperfine Interactions in Nitroaromatic Radical Anions	81
P. VAN HECKE, H. W. SPIESS, U. HAEBERLEN, AND S. HAUSSÜHL. NMR Study of a Single Crystal of KHF_2 . I. ^1H and ^{19}F Dipolar Spectra.	93
P. VAN HECKE, H. W. SPIESS, AND U. HAEBERLEN. NMR Study of a Single Crystal of KHF_2 . II. Proton Magnetic Shielding Tensor	103
ANTHONY J. MONTANA AND BENJAMIN P. DAILEY. NMR Studies of Spherical Molecules Dissolved in Smectic Liquid Crystal Solvents	117
OLA HARTMANN. Dipole-Dipole Relaxation in a Two-Spin System	125
CHING-HSIANG CHEN AND HAROLD W. DODGEN. Nuclear Quadrupole Resonance of Nitrogen-14 in Guanidine Complexes, Cyanoguanidine, and Substituted Ureas	139

COMMUNICATIONS

MICHAEL D. GORDON AND LOUIS D. QUIN. Temperature Dependence of ^{31}P NMR Chemical Shifts of Some Trivalent Phosphorus Compounds	149
R. E. SANTINI AND J. B. GRUTZNER. A Broadband System for the Observation of NMR Spectra of Any Resonant Nucleus	155
H. D. KIPNICH, R. ESCHÉ, AND W. MAURER. Improvement of the Normally Achievable Signal-to-Noise Ratio on a 270 MHz Spectrometer by Means of a Simple One-Step HF Preamplifier	161
R. A. ASSINK. A Quadrupole Coil for Nuclear Magnetic Resonance Spin-Echo Diffusion Measurements as a Function of Pressure	165
ANNOUNCEMENTS AND NEWS ITEMS	169

NUMBER 2, MAY 1976

SHULAMITH SCHLICK AND LARRY KEVAN. The Application of Differential Saturation to Distinguish Radial and Angular Modulation Mechanisms of Electron Spin-Lattice Relaxation.	171
PETER H. MCCABE AND CHARLES R. NELSON. Proton Chemical Shifts from Decoupled ^{13}C NMR Spectra	183
P. SAMBASIVA RAO AND S. SUBRAMANIAN. Jahn-Teller Tunneling in Copper(II)-Doped Hexaimidazole Zinc(II) Dichloride Tetrahydrate	191
M. DUCHÊNE, J. W. EMSLEY, J. C. LINDON, D. S. STEPHENSON, AND S. R. SALMAN. Structures of Some Fluorinated Pyridines from the Analysis of NMR Spectra of Nematic Solutions	207
T. PORUMB AND E. F. SLADE. A Computational Model for the Synthesis of ESR Spectra of Systems with One Axis of Symmetry	219
T. C. WONG AND E. E. BURNELL. A Nuclear Magnetic Resonance Study of Benzoyl Fluoride Partially Oriented in Nematic Phases: Molecular Structure, Barrier to Rotation, and Order Matrix	227
G. BALIMANN AND P. S. PREGOSIN. A Study of Phosphorus-Carbon Coupling Constants in Pd(II) and Pt(II) Phosphine Complexes	235
A. ROCKENBAUER AND P. SIMON. Ambiguity Problems of the Spin Hamiltonian.	243
S. I. PARKS AND R. B. JOHANNESSEN. An Algorithm for Automatic Correction of Quadrature Phase Detector Outputs	265
ARTHUR E. STILLMAN AND ROBERT N. SCHWARTZ. Heisenberg Exchange in Inhomogeneously Broadened Nitroxide EPR Spectra	269
LUDGER ERNST. ^{13}C NMR Spectroscopy of Polycyclic Aromatics VII. Naphthalenes Carrying Electron-Withdrawing Substituents. Correlations between Substituent-Induced Shifts and INDO MO Charge Densities	27

MYONG-KU AHN. Diffusion Coefficients of Paramagnetic Species in Solution.	289
M. J. HUNT AND A. L. MACKAY. Deuterium and Nitrogen Pure Quadrupole Resonance in Amino Acids. II	295
M. LIPSICAS, M. SIEGEL, J. PIOTT, T. HIGGINS, AND J. A. GERBER. Proton Spin-Lattice Relaxation in Some Paramagnetically Adulterated Hydrocarbon Gases	303
KARL-ÅKE THUOMAS AND ANDERS LUND. Analysis of EPR with Large Quadrupole Interaction	315
YOJI ARATA. Application of Correlation NMR Spectroscopy to CIDNP	327
F. CAVAGNA AND C. SCHUMANN. Non-Bond F-F Nuclear Spin Couplings. II. Hexafluoropropene Trimers	333
JAMES W. COOPER. Computers in NMR. II. Experimental Investigation of Noise and Dynamic Range in the Fourier Transform Process	345
P. KREBS AND E. SACKMANN. Triplet ESR Spectroscopy in Ordered Glasses. A Spectroscopic Application of Liquid Crystals.	359
BERNARD R. APPLEMAN AND BENJAMIN P. DAILEY. Carbon-13 Shielding Tensors of CCl_3X Systems from Studies of Liquid-Crystal Solutions	375
COMMUNICATIONS	
RUTH A. PICKERING AND PAUL V. ROLING. NMR Shift Reagents: A Stereoselective Interaction of $\text{Eu}(\text{TFN})_3$ with Methyl Ketones	385
FREDERICK W. KING AND H. BERNHARD SCHLEGEL. An <i>ab initio</i> Study of the Bicyclobutyl Radical: An <i>anti</i> -W Long-Range Coupled System	389
SOOK LEE AND I. M. BROWN. EPR Investigations of Peroxy Radicals in γ -Irradiated Poly(Methyl Methacrylate)	393
ERRATUM	397

NUMBER 3, JUNE 1976

B. P. LEMKE AND D. HANEMAN. Magnetic-Field-Induced Transitions in Magnetite Observed by EPR	399
P. GRANGER AND M. MAUGRAS. Long-Range ^{13}C -H Coupling Constants in Mono- and Diacetoxynaphthalenes	405
ROLF SJÖBLOM. A General Procedure for the Calculation of Theoretical Nuclear Magnetic Resonance Second Moments in Dipolar Solids; Application to Oxalic Acid Dihydrate	411

ROLF SJÖBLOM. A General Procedure for the Calculation of Theoretical Nuclear Magnetic Relaxation Times in Dipolar Solids; Applications to the Trimethylammonium Ion	425
N. C. VIZIA, P. N. MURTY, C. R. K. MURTY AND V. NAGARAJAN. NMR in Paramagnetic $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$ and $\text{LiCuCl}_3 \cdot 2\text{D}_2\text{O}$	439
J. F. HINTON AND R. W. BRIGGS. Thallium-205 NMR Spectroscopy. II. ^{205}Tl Chemical Shifts and Coupling Constants in Substituted Arylthallium(III)-bis(Trifluoroacetates)	447
FLAVIANO COLETTA, RENATO ETTORRE, AND ALESSANDRO GAMBARO. ^1H and ^{13}C NMR Studies of Palladium(II) and Platinum(II) Complexation of Cytosine	453
LUDGER ERNST, ERNEST LUSTIG, AND VICTOR WRAY. A ^1H , ^{13}C , and ^{15}N NMR Spectral Analysis of ^{15}N -Nitrobenzene	459
WILSON M. GULICK, JR. Barriers to Interconversion of Nonequivalent Methyl Groups in Tetrakis(dimethylamino)ethylene Dibromide and Two Closely Related Molecules	467
W. FREEMAN, P. S. PREGOSIN, S. N. SZE, AND L. M. VENANZI. Platinum-195 NMR Using Fourier Transform Techniques. The PtCl_4^{2-} Ion	473
NORBERT MULLER. Volume of Mixing Effect on Solvent Shifts in Fluorine Magnetic Resonance Spectra	479
J. J. WINDLE. Methods for Improving the Measurement and Control of Temperature in the Variable Temperature System of the Varian E-3 EPR Spectrometer	487
B. W. GOODWIN, R. WALLACE, AND R. K. HARRIS. Relaxation Studies Using Saturated Bandshapes in High-Resolution NMR. I. Symmetric Three Spin- $\frac{1}{2}$ Systems	491
DANIEL PINKEL AND SHELDON SCHULTZ. Geometrical Effects in Conduction Electron Spin Resonance in Metals	509
MILTON T. W. HEARN. Carbon-13 Nuclear Magnetic Resonance Spectra of <i>cis</i> - and <i>trans</i> -Alk-3-en-1-yne and Their 1-Trimethylsilyl Derivatives	521
M. PUNKKINEN, J. E. TUOHI, AND E. E. YLINEN. Proton Magnetic Resonance Spectrum of Tunneling Ammonium Ions	527
D. CANET, C. GOULON-GINET, AND J. P. MARCHAL. Accurate Determination of Parameters for ^{17}O in Natural Abundance by Fourier Transform NMR	537
J. L. BONARDET AND J. P. FRAISSARD. Method of Correcting Chemical Shifts of Adsorbate Molecules for Adsorbent Susceptibility	543
S. DUMITRU, I. INȚA, AND MARIA DUMITRU. Stationary Approximation for the Nonequilibrium Fluctuations in Paramagnetic Systems.	549

COMMUNICATIONS

- N. R. KRISHNA. A Method for Solvent Peak Suppression in FTNMR Spectra by Double Resonance 555
- D. I. HOULT AND R. E. RICHARDS. An Ultra High Frequency Receiver Protection Scheme 561


BOOK REVIEW

- "The Practice of NMR Spectroscopy, with Spectra-Structure Correlations for Hydrogen-1", by Nugent F. Chamberlain 565

ANNOUNCEMENTS AND NEWS ITEMS 567

AUTHOR INDEX for Volume 22 569

Subject Index for Volume 22 will appear in the December 1976 issue as part of a cumulative index for the year 1976.



Digitized by the Internet Archive
in 2023 with funding from
Kahle/Austin Foundation

Information for Authors

The *Journal of Magnetic Resonance* includes original papers, both full articles and communications, dealing with the theory, techniques, methods of spectral analysis and interpretation, spectral correlations, and results of magnetic resonance spectroscopy and related fields. Submission of a manuscript to the *Journal* implies that none of the content has been published or is under consideration for publication elsewhere, except as specifically indicated by the author. The Editor seeks the assistance of expert referees in the evaluation of manuscripts of articles, but he alone is responsible for the final decision concerning acceptance.

Communications are preliminary accounts of work of special importance or contain discussion of controversial subjects. Communications must be especially carefully and concisely prepared; since they may not be refereed, it is the responsibility of the author to ensure that the manuscript as originally submitted is free of typographical or substantive errors. To save time in publication, proofs of communications are not sent to the authors for correction.

Fifty reprints of each paper are supplied without charge, and additional reprints may be ordered on a form which is sent to the author. For articles, the reprint order form accompanies the galley proofs which the author receives. The *Journal assesses no page or publication charges*.

All manuscripts and books for review should be sent to the Editor, Wallace S. Brey, Department of Chemistry, University of Florida, Gainesville, Florida 32611.

Arrangement of the Paper

If the paper is lengthy, it should be divided into sections, although it is preferred that the sections not be numbered. Tables are numbered consecutively with *Arabic* numerals and are to be mentioned in order in the text. Each table should be supplied with a title. Figures are also numbered consecutively with *Arabic* numerals and are mentioned in order in the text. Each regular article requires an abstract which should describe concisely the substantive content, the conclusions reached, and the contributions of the research described. Since the abstract may be used directly by Chemical Abstracts and other abstracting services, it must be self-contained, having no references to formulas, equations, or bibliographic citations which appear in the body of the manuscript.

Literature references are cited in numerical order in the text by *in-line, parenthesized, italic numerals*. References to "unpublished" or "to be published" work from the author's laboratory should not be given. However, dissertations may be cited, or papers actually accepted may be referred to as "in press" if the name of the journal is included.

Authors are urged to give careful thought to the logical construction of the manuscript, so that explanatory or parenthetical footnotes need not be employed—where possible, such material should be incorporated in the text. Any footnotes which are indispensable are not intermixed with references, but are indicated in the text by consecutive, superscript numerals, and each footnote will then appear in print at the bottom of the page on which it is cited. Equation numbers are given in *square* brackets to the right of the equation, and references in the text to equations should be in the form "Eq. [3]."

Form of Manuscript

Manuscripts should be submitted in triplicate. The *original typewritten copy* should be supplied; mimeo, electrostatic, and similar process reproductions are not usually sufficiently clear. All of the typing must be *double-spaced*, including that of abstract, references, and footnotes, on one side of good quality paper approximately 22 × 28 cm (8.5 × 11 in.) in dimensions. The first line of each paragraph is indented.

Each page of the manuscript should be numbered. The first page contains the article title, the author's name, and affiliation. At the bottom of this page should appear any footnotes to the title (indicated by superscript *, †, ‡); the number of manuscript pages, figures, and tables should also be noted. The second page should contain the abstract of 50–200 words.

Symbols and Abbreviations. The American Chemical Society's Handbook for Authors, 1967 edition, or the Style Manual of the American Institute of Physics should be followed for standard abbreviations, names, and symbols for units. Mathematical equations or symbols must be typewritten whenever possible. Greek letters may be identified in pencil in the margin. The author of any manuscript in

which there are mathematical equations or symbols is urged to supply a list of these on a separate sheet for the assistance of the printer in selecting the proper type. The list will not appear in print.

References and Footnotes. References to the literature should be cited in order in the text by in-line, parenthesized numerals. The references themselves are to be typed double-spaced on a separate sheet in numerical order. Each reference contains the author's initials, last name, journal name, volume, initial page number, and year in parentheses, *in that order*. The name of the journal is abbreviated in the style of Chemical Abstracts' *Service Source Index* (1969 Edition). For book references, the form is author's name, name of the book in quotation marks, editor's name (if any), edition if other than the first, chapter or page number, publisher's name, place of publication, and year of publication.

Any footnotes which are included are numbered in a sequence separate from the references and must be typed in the manuscript on a separate page.

Tables. Tables should be laid out carefully, so that minimum space is used and entries are accurately grouped and clearly labeled. Usually, a table should be arranged vertically, with more rows than columns. Vertical lines are not used to separate the columns. Each table is numbered with an Arabic numeral, provided with a title, and typed on a separate sheet of paper. Footnotes to the table are placed directly below it and are indicated by superscript, lower-case, italic letters (^a, ^b, ^c). Tables that are longer than two manuscript pages will be reproduced photographically, and should therefore be typed in the exact form desired. All such tables should be carefully checked since errors cannot be corrected in proof.

Figures. Figures must be carefully drawn in black, waterproof drawing ink, to draftsman's standards, with lettering by stencil or drawing machine. Freehand, penciled, or typewritten lettering is not acceptable. Lettering should include numerical scales and units required for the two axes, and should be large enough to be legible after reduction by 50–60%. The illustration copy should be on sheets of the same size as that on which the manuscript is typed. Smaller figures may be mounted on sheets of the required size, and larger originals may be handled by supplying glossy, high-contrast, photographic reductions. The original and two duplicates of each figure are required.

Diagrams. Ink drawings should be supplied for any complex molecular formulas or diagrams involving material which the printer cannot readily set in type.

Proofs. Galley proofs will be sent to the author with reprint order forms. Fifty reprints of each article will be supplied free of charge.